

## AMENDMENTS TO THE CLAIMS

1 (currently amended). A method of providing a representative, non-redundant overview of the peptide content of a sample type by analyzing a plurality of samples using its peptide topology, wherein the method comprises the steps of:

- a) providing a respective mass spectrum for each sample of said plurality of samples, wherein signal intensity peaks correspond to potential peptides,
- b) computing ~~the~~ measures of correlation between the signal ~~intensities~~ intensity peaks of said potential peptides,
- c) grouping potential peptides together, which exhibit a degree of correlation among each other above a certain threshold, thereby providing a plurality of correlation associated networks of potential peptides, and
- d) assigning at least one ~~representative~~ potential peptide out of at least one correlation associated network as a representative peptide to said correlation associated network of said sample type.

2 (currently amended). A method for predicting the amino acid sequence of peptides using the peptide topology of a plurality of samples containing a peptide having a known precursor, wherein the method comprises the steps of:

- a) providing a respective mass spectrum for each sample of said plurality of samples, wherein signal intensity peaks correspond to potential peptides,
- b) identifying said peptide having a known precursor using the mass ~~of said peptide thereof~~, wherein the sequence of the known precursor is known,
- c) computing ~~the~~ measures of correlation between the signal intensity of said peptide having a known precursor and ~~the~~ signal intensities of ~~the~~ other potential peptides in each sample,
- d) selecting potential peptides, which exhibit a degree of correlation with said peptide having a known precursor above a certain threshold, and
- e) predicting ~~the~~ a sequence for ~~of~~ the potential peptides selected in step d) by matching masses of putative fragments of the sequence of the known precursor with ~~the~~ masses of the

potential peptides correlating with said peptide having a known precursor.

3 (currently amended). A method for predicting the sequence of peptides using the peptide topology of a plurality of samples containing a known peptide with a known sequence, wherein the method comprises the steps of:

- a) providing a respective mass spectrum for each sample of said plurality of samples, wherein signal intensity peaks correspond to potential peptides,
- b) identifying a peptide with a known sequence in said plurality of samples using ~~it's~~ the mass of said peptide with a known sequence,
- c) computing ~~the~~ measures of correlation between the signal intensity of said known peptide and ~~the~~ signal intensities of the potential peptides,
- d) selecting potential peptides, which exhibit a degree of correlation with the known peptide above a certain threshold,
- e) computing ~~the~~ mass differences between each of the potential peptides and the known peptide, and
- f) predicting ~~the~~ a sequence and/or ~~the~~ a biologically, chemically or physically modified sequence of the potential peptides by using data about mass differences caused by biological, chemical or physical processes matching the mass differences ~~determined~~ computed in step e).

4 (currently amended). A method for identifying peptides suitable to be used as marker panels using the peptide topology of a plurality of samples taken from at least two different experimental groups representing a status A and a status B, wherein the method comprises the steps of:

- a) providing a respective mass spectrum for each sample of said plurality of samples, wherein signal intensity peaks correspond to potential peptides,
- b) computing ~~the~~ measures of correlation between the signal intensities of said potential peptides for each sample of the plurality of samples within each experimental group separately, and
- c) selecting pairs of potential peptides, which exhibit a difference in ~~the~~ degree of correlation between the different experimental groups above a certain threshold, thereby

providing peptides which are suitable to be used as marker panels for diagnostic purposes to distinguish between status A and status B.

5 (currently amended). A method for identifying peptides suitable to be used as marker panels using the peptide topology of a plurality of samples taken from at least two different experimental groups representing a status A and a status B, wherein the method comprises the steps of:

- a) providing a respective mass spectrum for each sample of said plurality of samples, wherein signal intensity peaks correspond to potential peptides,
- b) selecting potential peptides correlating with a parameter being representative of status A or status B,
- c) computing ~~the~~ measures of correlation between ~~the~~ signal intensities of said selected potential peptides for each plurality of samples, and
- d) selecting pairs of potential peptides which exhibit no correlation of their respective signal intensities above a certain threshold, thereby providing potential peptides which are suitable to be used as complementing peptides in a marker panel for diagnostic purposes to distinguish between status A and status B.

6 (currently amended). A method for identifying peptides suitable as a surrogate for a known peptide using the peptide topology of a plurality of samples, wherein the method comprises the steps of:

- a) providing a respective mass spectrum for each sample of said plurality of samples, wherein signal intensity peaks correspond to potential peptides,
- b) computing ~~the~~ measures of correlation between the signal intensity of said known peptide and ~~the~~ signal intensities of the potential peptides, and
- c) selecting potential peptides, which exhibit a degree of correlation with said known peptide above a certain threshold, thereby providing potential peptides suitable as a surrogate for said known peptide.

7 (currently amended). The method according to ~~any one of claims 1 to 3 or 6~~ claim 1,

where a plurality of minimal spanning tree diameters is computed as a measure of correlation using the signal intensity of each of said potential peptides in said plurality of samples, wherein the selection of potential peptides is done by using a minimal spanning tree diameter threshold, wherein the minimal spanning tree diameter for an association of two potential peptides ~~has to be~~ is above an adjustable threshold of at least 0.425 times the number of samples.

8 (currently amended). The method according to ~~claims 4 or 5~~ claim 4, where a plurality of minimal spanning tree diameters is computed as a measure of correlation using the signal intensity of said potential peptides in said plurality of samples, wherein the selection of pairs of potential peptides is done by using a minimal spanning tree diameter threshold, wherein ~~the difference between~~ the minimal spanning tree ~~diameter~~ diameters found in the said different experimental groups differ by an amount that is above an adjustable threshold of at least 0.1 times the number of samples.

9 (currently amended). The method according to ~~any one of the preceding claims~~ claim 1, wherein the method comprises the additional step of ~~at least one~~ fractionating step of each sample of said plurality of samples prior to providing the mass ~~spectra of said samples~~ spectrum of each sample and wherein at least one fraction ~~of said samples~~ obtained by said fractionating is used for providing said mass ~~spectra~~ spectrum for each sample.

10 (currently amended). The method according to ~~any one of the preceding claims~~ claim 1 using at least one measure of correlation selected from the group consisting of "Pearson Product-Moment Correlation Coefficient", "Spearman's rank order Correlation Coefficient", "Kendall's Tau", "Kendall's Coefficient of Concordance", "Goodman and Kruskal's Gamma" and "Minimal Spanning Tree diameters".

11 (currently amended). The method according to ~~any one of the preceding claims~~ claim 1 using at least one method for calibrating ~~the~~ mass spectrometric data selected from the group consisting of "Simple Offset Correction", "2-Point Baseline Correction", "Multi-Point Baseline Correction", "Interactive Polynomial Baseline Correction", "Function Fit Baseline Correction",

and"GIFTS (Auto Leveling Method) Baseline Correction".

12 (currently amended). The method according to ~~any one of the preceding claims~~ claim 1 using at least one method for identifying outlier samples selected from the group consisting of "Principal Component Analysis", "multivariate calibration partial least-squares", and "Replicator Neural Networks".

13 (currently amended). The method according to ~~any one of the preceding claims~~ claim 1, wherein ~~the calculation of the step of calculating~~ the measures of correlation is repeated at least once using the peptide coordinates resulting from the a previous round of calculations of measures of correlation, thereby providing the measures of correlation of 2<sup>nd</sup> or higher order ~~neighborhood~~.

14 (currently amended). The method according to ~~any one of the preceding claims~~ claim 1 using additional coordinates data besides the mass signal intensity to compute the measures of correlation, the additional data being selected from the group consisting of fraction number, elution time, retention time, protein chip coordinates, peptide concentration, enzyme activities, structural properties, chemical properties and biological properties.

15 (currently amended). The method according to ~~any one of the preceding claims~~ claim 1, wherein MALDI mass spectrometry or ESI mass spectrometry is used to generate the mass ~~spectra~~ spectrum of each sample.

16 (currently amended). The method according to ~~any one of the preceding claims~~ claim 1, wherein ~~the samples or groups of samples are~~ each sample of the plurality of samples is homogeneous.

17 (currently amended). The method according to ~~any one of the preceding claims~~ claim 1, wherein the ~~computation of measures of correlation is done in advance prior to the analysis to accelerate the speed of the analysis using~~ pre-determined values for the measures of correlation

are utilized in step b).

18 (currently amended). The method according to ~~any one of the preceding claims~~ claim 1, wherein ~~the necessary~~ sequence information corresponding to a mass spectral peak is provided by manual input or automatically queried from a database.

19 (currently amended). The method according to ~~any one of the preceding claims~~ claim 1, wherein ~~the corresponding results are automatically combined with~~ data from other sources is automatically combined with the signal intensity to aid in assigning the representative peptide; ~~chosen~~ the other sources being selected from the group consisting of sequence databases, patent databases, literature databases, medical databases, 3D structure databases, and databases containing information about enzyme recognition sites, posttranslational modifications, genetic polymorphisms, and clinical trials.

20 (currently amended). The method according to ~~any one of the preceding claims~~ claim 1, wherein at least one step ~~of data processing or data supply is done~~ or a portion thereof is performed using a remote computer system and wherein ~~the~~ a user is connected via an internet, intranet or other network to the remote computer system.

21 (currently amended). A digital computer system programmed to perform a method according to ~~any one of the preceding claims~~ claim 1.

22 (currently amended). A computer readable medium storing a computer program implementing a method according to ~~any one of claims 1 to 20~~ claim 1.

23 (currently amended). ~~Use of a~~ The method according to ~~any one of the previous claims~~ claim 1, wherein at least ~~part of the data-analysis~~ one step or a portion thereof is done via is performed utilizing a remote computer system located in a different country.

24 (currently amended). ~~Use of a~~ The method according to ~~any one of claims 2,3 and 6 to~~

~~23 claim 2 for further comprising determining alterations~~ an alteration in the amino acid sequence length and/or for determining chemical or posttranslational modifications of peptides of a peptide of known identity ~~which peptides were added to the~~ a sample of the plurality of samples.

25 (new). The method according to claim 2, wherein a plurality of minimal spanning tree diameters is computed as a measure of correlation using the signal intensity of each of said potential peptides in said plurality of samples, wherein the selection of potential peptides is done by using a minimal spanning tree diameter threshold, wherein the minimal spanning tree diameter for an association of two potential peptides is above an adjustable threshold of at least 0.425 times the number of samples.

26 (new). The method according to claim 2, wherein the method comprises the additional step of fractionating each sample of said plurality of samples prior to providing the mass spectrum of each sample and wherein at least one fraction obtained by said fractionating is used for providing said mass spectrum for each sample.

27 (new). The method according to claim 2 using at least one measure of correlation selected from the group consisting of "Pearson Product-Moment Correlation Coefficient", "Spearman's rank order Correlation Coefficient", "Kendall's Tau", "Kendall's Coefficient of Concordance", "Goodman and Kruskal's Gamma" and "Minimal Spanning Tree diameters".

28 (new). The method according to claim 2 using at least one method for calibrating mass spectrometric data selected from the group consisting of "Simple Offset Correction", "2-Point Baseline Correction", "Multi-Point Baseline Correction", "Interactive Polynomial Baseline Correction", "Function Fit Baseline Correction", and "GIFTS (Auto Leveling Method) Baseline Correction".

29 (new). The method according to claim 2 using at least one method for identifying outlier samples selected from the group consisting of "Principal Component

Analysis", "multivariate calibration partial least-squares", and "Replicator Neural Networks".

30 (new). The method according to claim 2, wherein the step of calculating of the measures of correlation is repeated at least once using peptide coordinates resulting from a previous round of calculating measures of correlation, thereby providing measures of correlation of 2<sup>nd</sup> or higher order.

31 (new). The method according to claim 2 using additional data besides signal intensity to compute the measures of correlation, the additional data being selected from the group consisting of fraction number, elution time, retention time, protein chip coordinates, peptide concentration, enzyme activities, structural properties, chemical properties and biological properties.

32 (new). The method according to claim 2, wherein MALDI mass spectrometry or ESI mass spectrometry is used to generate the mass spectrum of each sample.

33 (new). The method according to claim 2, wherein each sample of the plurality of samples is homogeneous.

34 (new). The method according to claim 2, wherein pre-determined values for the measures of correlation are utilized in step c).

35 (new). The method according to claim 2, wherein sequence information corresponding to a mass spectral peak is provided by manual input or automatically queried from a database.

36 (new). The method according to claim 2, wherein data from other sources is automatically combined with the signal intensity to aid in assigning the representative peptide; the other sources being selected from the group consisting of sequence databases, patent databases, literature databases, medical databases, 3D structure databases, and databases



containing information about enzyme recognition sites, posttranslational modifications, genetic polymorphisms, and clinical trials.

37 (new). The method according to claim 2, wherein at least one step or a portion thereof is performed using a remote computer system and wherein a user is connected via an internet, intranet or other network to the remote computer system.

38 (new). A digital computer system programmed to perform a method according to claim 2.

39 (new). A computer readable medium storing a computer program implementing a method according to claim 2.

40 (new). The method according to claim 2, wherein at least one step or a portion thereof is performed utilizing a remote computer system located in a different country.

41 (new). The method according to claim 3, wherein a plurality of minimal spanning tree diameters is computed as a measure of correlation using the signal intensity of each of said potential peptides in said plurality of samples, wherein the selection of potential peptides is done by using a minimal spanning tree diameter threshold, wherein the minimal spanning tree diameter for an association of two potential peptides is above an adjustable threshold of at least 0.425 times the number of samples.

42 (new). The method according to claim 3 further comprising determining an alteration in the amino acid sequence of a peptide of known identity added to a sample of the plurality of samples.

43 (new). The method according to claim 3, wherein the method comprises the additional step of fractionating each sample of said plurality of samples prior to providing the mass spectrum of each sample and wherein at least one fraction obtained by said fractionating is used

for providing said mass spectrum for each sample.

44 (new). The method according to claim 3 using at least one measure of correlation selected from the group consisting of "Pearson Product-Moment Correlation Coefficient", "Spearman's rank order Correlation Coefficient", "Kendall's Tau", "Kendall's Coefficient of Concordance", "Goodman and Kruskal's Gamma" and "Minimal Spanning Tree diameters".

45 (new). The method according to claim 3 using at least one method for calibrating mass spectrometric data selected from the group consisting of "Simple Offset Correction", "2-Point Baseline Correction", "Multi-Point Baseline Correction", "Interactive Polynomial Baseline Correction", "Function Fit Baseline Correction", and "GIFTS (Auto Leveling Method) Baseline Correction".

46 (new). The method according to claim 3 using at least one method for identifying outlier samples selected from the group consisting of "Principal Component Analysis", "multivariate calibration partial least-squares", and "Replicator Neural Networks".

47 (new). The method according to claim 3, wherein the step of calculating of the measures of correlation is repeated at least once using peptide coordinates resulting from a previous round of calculating measures of correlation, thereby providing measures of correlation of 2<sup>nd</sup> or higher order.

48 (new). The method according to claim 3 using additional data besides signal intensity to compute the measures of correlation, the additional data being selected from the group consisting of fraction number, elution time, retention time, protein chip coordinates, peptide concentration, enzyme activities, structural properties, chemical properties and biological properties.

49 (new). The method according to claim 3, wherein MALDI mass spectrometry or ESI mass spectrometry is used to generate the mass spectrum of each sample.

50 (new). The method according to claim 3, wherein each sample of the plurality of samples is homogeneous.

51 (new). The method according to claim 3, wherein pre-determined values for the measures of correlation are utilized in step d).

52(new). The method according to claim 3, wherein sequence information corresponding to a mass spectral peak is provided by manual input or automatically queried from a database.

53 (new). The method according to claim 3, wherein data from other sources is automatically combined with the signal intensity to aid in assigning the representative peptide; the other sources being selected from the group consisting of sequence databases, patent databases, literature databases, medical databases, 3D structure databases, and databases containing information about enzyme recognition sites, posttranslational modifications, genetic polymorphisms, and clinical trials.

54 (new). The method according to claim 3, wherein at least one step or a portion thereof is performed using a remote computer system and wherein a user is connected via an internet, intranet or other network to the remote computer system.

55 (new). A digital computer system programmed to perform a method according to claim 3.

56 (new). A computer readable medium storing a computer program implementing a method according to claim 3.

57 (new). The method according to claim 3, wherein at least one step or a portion thereof is performed utilizing a remote computer system located in a different country.

58 (new). The method according to claim 4, wherein the method comprises the additional

step of fractionating each sample of said plurality of samples prior to providing the mass spectrum of each sample and wherein at least one fraction obtained by said fractionating is used for providing said mass spectrum for each sample.

59 (new). The method according to claim 4 using at least one measure of correlation selected from the group consisting of "Pearson Product-Moment Correlation Coefficient", "Spearman's rank order Correlation Coefficient", "Kendall's Tau", "Kendall's Coefficient of Concordance", "Goodman and Kruskal's Gamma" and "Minimal Spanning Tree diameters".

60 (new). The method according to claim 4 using at least one method for calibrating mass spectrometric data selected from the group consisting of "Simple Offset Correction", "2-Point Baseline Correction", "Multi-Point Baseline Correction", "Interactive Polynomial Baseline Correction", "Function Fit Baseline Correction", and "GIFTS (Auto Leveling Method) Baseline Correction".

61 (new). The method according to claim 4 using at least one method for identifying outlier samples selected from the group consisting of "Principal Component Analysis", "multivariate calibration partial least-squares", and "Replicator Neural Networks".

62 (new). The method according to claim 4, wherein the step of calculating of the measures of correlation is repeated at least once using peptide coordinates resulting from a previous round of calculating measures of correlation, thereby providing measures of correlation of 2<sup>nd</sup> or higher order.

63 (new). The method according to claim 4 using additional data besides signal intensity to compute the measures of correlation, the additional data being selected from the group consisting of fraction number, elution time, retention time, protein chip coordinates, peptide concentration, enzyme activities, structural properties, chemical properties and biological properties.

64 (new). The method according to claim 4, wherein MALDI mass spectrometry or ESI mass spectrometry is used to generate the mass spectrum of each sample.

65 (new). The method according to claim 4, wherein each sample of the plurality of samples is homogeneous.

66 (new). The method according to claim 4, wherein pre-determined values for the measures of correlation are utilized in step c).

67 (new). The method according to claim 4, wherein sequence information corresponding to a mass spectral peak is provided by manual input or automatically queried from a database.

68 (new). The method according to claim 4, wherein data from other sources is automatically combined with the signal intensity to aid in assigning the representative peptide; the other sources being selected from the group consisting of sequence databases, patent databases, literature databases, medical databases, 3D structure databases, and databases containing information about enzyme recognition sites, posttranslational modifications, genetic polymorphisms, and clinical trials.

69 (new). The method according to claim 4, wherein at least one step or a portion thereof is performed using a remote computer system and wherein a user is connected via an internet, intranet or other network to the remote computer system.

70 (new). A digital computer system programmed to perform a method according to claim 4.

71 (new). A computer readable medium storing a computer program implementing a method according to claim 4.

72 (new). The method according to claim 4, wherein at least one step or a portion thereof is performed utilizing a remote computer system located in a different country.

73 (new). The method according to claim 5, wherein a plurality of minimal spanning tree diameters is computed as a measure of correlation using the signal intensity of said potential peptides in said plurality of samples, wherein the selection of pairs of potential peptides is done by using a minimal spanning tree diameter threshold, wherein the minimal spanning tree diameters found in the said different experimental groups differ by an amount that is above an adjustable threshold of at least 0.1 times the number of samples.

74 (new). The method according to claim 5, wherein the method comprises the additional step of fractionating each sample of said plurality of samples prior to providing the mass spectrum of each sample and wherein at least one fraction obtained by said fractionating is used for providing said mass spectrum for each sample.

75 (new). The method according to claim 5 using at least one measure of correlation selected from the group consisting of "Pearson Product-Moment Correlation Coefficient", "Spearman's rank order Correlation Coefficient", "Kendall's Tau", "Kendall's Coefficient of Concordance", "Goodman and Kruskal's Gamma" and "Minimal Spanning Tree diameters".

76 (new). The method according to claim 5 using at least one method for calibrating mass spectrometric data selected from the group consisting of "Simple Offset Correction", "2-Point Baseline Correction", "Multi-Point Baseline Correction", "Interactive Polynomial Baseline Correction", "Function Fit Baseline Correction", and "GIFTS (Auto Leveling Method) Baseline Correction".

77 (new). The method according to claim 5 using at least one method for identifying outlier samples selected from the group consisting of "Principal Component Analysis", "multivariate calibration partial least-squares", and "Replicator Neural Networks".

78 (new). The method according to claim 5, wherein the step of calculating of the measures of correlation is repeated at least once using peptide coordinates resulting from a previous round of calculating measures of correlation, thereby providing measures of correlation of 2<sup>nd</sup> or higher order.

79 (new). The method according to claim 5 using additional data besides signal intensity to compute the measures of correlation, the additional data being selected from the group consisting of fraction number, elution time, retention time, protein chip coordinates, peptide concentration, enzyme activities, structural properties, chemical properties and biological properties.

80 (new). The method according to claim 5, wherein MALDI mass spectrometry or ESI mass spectrometry is used to generate the mass spectrum of each sample.

81 (new). The method according to claim 5, wherein each sample of the plurality of samples is homogeneous.

82 (new). The method according to claim 5, wherein pre-determined values for the measures of correlation are utilized in step d).

83 (new). The method according to claim 5, wherein sequence information corresponding to a mass spectral peak is provided by manual input or automatically queried from a database.

84 (new). The method according to claim 5, wherein data from other sources is automatically combined with the signal intensity to aid in assigning the representative peptide; the other sources being selected from the group consisting of sequence databases, patent databases, literature databases, medical databases, 3D structure databases, and databases containing information about enzyme recognition sites, posttranslational modifications, genetic polymorphisms, and clinical trials.

85 (new). The method according to claim 5, wherein at least one step or a portion thereof is performed using a remote computer system and wherein a user is connected via an internet, intranet or other network to the remote computer system.

86 (new). A digital computer system programmed to perform a method according to claim 5.

87 (new). A computer readable medium storing a computer program implementing a method according to claim 5.

88 (new). The method according to claim 5, wherein at least one step or a portion thereof is performed utilizing a remote computer system located in a different country.

89 (new). The method according to claim 6, wherein a plurality of minimal spanning tree diameters is computed as a measure of correlation using the signal intensity of each of said potential peptides in said plurality of samples, wherein the selection of potential peptides is done by using a minimal spanning tree diameter threshold, wherein the minimal spanning tree diameter for an association of two potential peptides is above an adjustable threshold of at least 0.425 times the number of samples.

90 (new). The method according to claim 6 further comprising determining an alteration in the amino acid sequence of a peptide of known identity added to a sample of the plurality of samples.

91 (new). The method according to claim 6, wherein the method comprises the additional step of fractionating each sample of said plurality of samples prior to providing the mass spectrum of each sample and wherein at least one fraction obtained by said fractionating is used for providing said mass spectrum for each sample.

92 (new). The method according to claim 6 using at least one measure of correlation



selected from the group consisting of "Pearson Product-Moment Correlation Coefficient", "Spearman's rank order Correlation Coefficient", "Kendall's Tau", "Kendall's Coefficient of Concordance", "Goodman and Kruskal's Gamma" and "Minimal Spanning Tree diameters".

93 (new). The method according to claim 6 using at least one method for calibrating mass spectrometric data selected from the group consisting of "Simple Offset Correction", "2-Point Baseline Correction", "Multi-Point Baseline Correction", "Interactive Polynomial Baseline Correction", "Function Fit Baseline Correction", and "GIFTS (Auto , Leveling Method) Baseline Correction".

94 (new). The method according to claim 6 using at least one method for identifying outlier samples selected from the group consisting of "Principal Component Analysis", "multivariate calibration partial least-squares", and "Replicator Neural Networks".

95 (new). The method according to claim 6, wherein the step of calculating of the measures of correlation is repeated at least once using peptide coordinates resulting from a previous round of calculating measures of correlation, thereby providing measures of correlation of 2<sup>nd</sup> or higher order.

96 (new). The method according to claim 6 using additional data besides signal intensity to compute the measures of correlation, the additional data being selected from the group consisting of fraction number, elution time, retention time, protein chip coordinates, peptide concentration, enzyme activities, structural properties, chemical properties and biological properties.

97 (new). The method according to claim 6, wherein MALDI mass spectrometry or ESI mass spectrometry is used to generate the mass spectrum of each sample.

98 (new). The method according to claim 6, wherein each sample of the plurality of samples is homogeneous.

99 (new). The method according to claim 6, wherein pre-determined values for the measures of correlation are utilized in step c).

100 (new). The method according to claim 6, wherein sequence information corresponding to a mass spectral peak is provided by manual input or automatically queried from a database.

101 (new). The method according to claim 6, wherein data from other sources is automatically combined with the signal intensity to aid in assigning the representative peptide; the other sources being selected from the group consisting of sequence databases, patent databases, literature databases, medical databases, 3D structure databases, and databases containing information about enzyme recognition sites, posttranslational modifications, genetic polymorphisms, and clinical trials.

102 (new). The method according to claim 6, wherein at least one step or a portion thereof is performed using a remote computer system and wherein a user is connected via an internet, intranet or other network to the remote computer system.

103 (new). A digital computer system programmed to perform a method according to claim 6.

104 (new). A computer readable medium storing a computer program implementing a method according to claim 6.

105 (new). The method according to claim 6, wherein at least one step or a portion thereof is performed utilizing a remote computer system located in a different country.